

# Diglycolic acid, isobutyl 3-methylpent-2-yl ester

Inchi:	InChI=1S/C14H26O5/c1-6-11(4)12(5)19-14(16)9-17-8-13(15)18-7-10(2)3/h10-12H,6-9H2
InchiKey:	RMBCOTHZTPVOKR-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CCC(C)C(C)OC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	274.35

## Physical Properties

Property code	Value	Unit	Source
gf	-513.16	kJ/mol	Joback Method
hf	-969.95	kJ/mol	Joback Method
hfus	28.21	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.180		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	693.40	K	Joback Method
tc	876.67	K	Joback Method
tf	369.09	K	Joback Method
vc	0.868	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.44	J/molxK	693.40	Joback Method
cpg	668.59	J/molxK	723.94	Joback Method
cpg	683.92	J/molxK	754.49	Joback Method
cpg	698.42	J/molxK	785.03	Joback Method
cpg	712.09	J/molxK	815.58	Joback Method
cpg	724.93	J/molxK	846.12	Joback Method
cpg	736.93	J/molxK	876.67	Joback Method
dvisc	0.0019713	Paxs	369.09	Joback Method

dvisc	0.0008014	Paxs	423.14	Joback Method
dvisc	0.0003995	Paxs	477.19	Joback Method
dvisc	0.0002294	Paxs	531.25	Joback Method
dvisc	0.0001460	Paxs	585.30	Joback Method
dvisc	0.0001003	Paxs	639.35	Joback Method
dvisc	0.0000730	Paxs	693.40	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381871&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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